Pentyl acetate

628-63-7 | DTXSID1027263

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.44e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 9.23e-01

Confidence level: 9.02e-01

Nearest Neighbors from the Training Set

Image not found
Pentyl acetate
Measured: 1.32e-02
Predicted: 1.44e-02

Image not found
3-Methylbutyl acetate
Measured: 1.54e-02
Predicted: 1.47e-02

Image not found
Ethyl valerate
Measured: 1.70e-02
Predicted: 1.54e-02

Image not found
Ethyl isovalerate
Measured: 1.85e-02
Predicted: 1.54e-02

Image not found
Methyl hexanoate
Measured: 1.02e-02
Predicted: 1.36e-02